

Date : 2024-07-19

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24G05-PTH04

Customer Identification : Lemongrass - India - L80116R

Type : Essential Oil

Source : *Cymbopogon flexuosus*

Customer : Plant Therapy

Checked and approved by:

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

***ISO**

Results : See analysis summary (next page)

Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005

Date : 2024-07-17

PHYSICOCHEMICAL DATA

Refractive index : 1.4852 ± 0.0003 (20 °C)

Method : PC-MAT-016 - Measure of the refractive index of a liquid.

Analyst : Cindy Caron B. Sc.

Date : 2024-07-08

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY - CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
2-Methyl-3-buten-2-ol	0.03	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
Hexanal	0.01	Aliphatic aldehyde
Unknown	tr	Unknown
4-Heptanone	0.02	Aliphatic ketone
Tricyclene	0.13	Monoterpene
α -Pinene	0.18	Monoterpene
Camphene	1.03	Monoterpene
Sabinene	0.02	Monoterpene
β -Pinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.94	Aliphatic ketone
Myrcene	0.09	Monoterpene
6-Methyl-5-hepten-2-ol	0.08	Aliphatic alcohol
Octanal	0.07	Aliphatic aldehyde
α -Phellandrene	0.01	Monoterpene
<i>para</i> -Cymene	0.01	Monoterpene
1,8-Cineole	0.05	Monoterpenic ether
Limonene	0.68	Monoterpene
(<i>Z</i>)- β -Ocimene	0.32	Monoterpene
(<i>E</i>)- β -Ocimene	0.19	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.04	Aliphatic aldehyde
γ -Terpinene	0.01	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanone	1.10	Aliphatic ketone
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.05	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
4-Nonanol	0.03	Aliphatic alcohol
Rosefuran	0.13	Monoterpenic ether
Perillene	0.03	Monoterpenic ether
<i>cis</i> -Chrysanthemal?	0.10	Monoterpenic aldehyde
Linalool	1.05	Monoterpenic alcohol
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	0.04	Aliphatic ketone
<i>trans-para</i> -Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
Unknown	0.09	Unknown
Unknown	0.13	Unknown
Unknown	0.01	Unknown
<i>trans-para</i> -Menth-2-en-1-ol	0.01	Monoterpenic alcohol

<i>trans</i> -Chrysanthemal	0.29	Monoterpenic aldehyde
exo-Isocitral	0.07	Monoterpenic aldehyde
Citronellal	0.24	Monoterpenic aldehyde
Borneol	0.15	Monoterpenic alcohol
Isoneral	0.63	Monoterpenic aldehyde
α -Phellandren-8-ol	0.16	Monoterpenic alcohol
Terpinen-4-ol	[0.26]	Monoterpenic alcohol
Rosefuran oxide	[0.26]	Monoterpenic ether
Unknown	0.10	Oxygenated monoterpene
Unknown	0.54	Unknown
Isogeranial	0.71	Monoterpenic aldehyde
α -Terpineol	0.14	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
(4Z)-Decenal	0.08	Aliphatic aldehyde
Unknown	0.06	Unknown
<i>trans</i> -Isopiperitenol	0.07	Monoterpenic alcohol
Unknown	0.07	Oxygenated monoterpene
Decanal	0.18	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.01	Monoterpenic alcohol
2,3-Epoxyneral?	0.05	Monoterpenic aldehyde
Nerol	0.27	Monoterpenic alcohol
Citronellol	0.12	Monoterpenic alcohol
Neral	31.73	Monoterpenic aldehyde
Piperitone	0.05	Monoterpenic ketone
Geraniol	5.98	Monoterpenic alcohol
Geranial	41.57	Monoterpenic aldehyde
Bornyl acetate	0.35	Monoterpenic ester
Unknown	0.02	Oxygenated monoterpene
Geranyl formate	0.04	Monoterpenic ester
Methyl geranate	0.07	Monoterpenic ester
Unknown	0.05	Unknown
α -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.03	Monoterpenic ester
Cyclosativene I	0.07	Sesquiterpene
Cyclosativene II	0.08	Sesquiterpene
α -Copaene	0.04	Sesquiterpene
Geranic acid	0.27	Aliphatic acid
β -Bourbonene	0.04	Sesquiterpene
Geranyl acetate	2.83	Monoterpenic ester
β -Elemene	0.08	Sesquiterpene
Longifolene	0.03	Sesquiterpene
β -Ylangene	0.08	Sesquiterpene
β -Caryophyllene	1.12	Sesquiterpene
β -Copaene	0.03	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.02	Sesquiterpene

6,9-Guaiadiene	0.03	Sesquiterpene
<i>cis</i> - β -Bergamotene?	0.02	Sesquiterpene
α -Humulene	0.14	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.36	Phenylpropanoid
<i>cis</i> -Muurolo-4(15),5-diene	0.04	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.03	Sesquiterpene
Germacrene D	0.17	Sesquiterpene
γ -Amorphene	0.03	Sesquiterpene
epi-Cubebol	0.11	Sesquiterpenic alcohol
α -Muurolole	0.04	Sesquiterpene
Methyl (<i>E</i>)-isoeugenol	0.02	Phenylpropanoid
δ -Amorphene	0.02	Sesquiterpene
γ -Cadinene	1.09	Sesquiterpene
Cubebol	0.18	Sesquiterpenic alcohol
δ -Cadinene	0.24	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.02	Sesquiterpene
10-epi-Cubebol?	0.03	Sesquiterpenic alcohol
(<i>E</i>)- γ -Bisabolene	0.08	Sesquiterpene
Unknown	0.04	Unknown
α -Cadinene	0.05	Sesquiterpene
Neryl butyrate	0.03	Monoterpenic ester
α -Elemol	0.04	Sesquiterpenic alcohol
Germacrene B	0.03	Sesquiterpene
Geranyl butyrate	0.09	Monoterpenic ester
Caryophyllene oxide	0.49	Sesquiterpenic ether
Caryophyllene oxide isomer	0.03	Sesquiterpenic ether
Humulene epoxide II	0.05	Sesquiterpenic ether
Selin-6-en-4 α -ol isomer	0.03	Sesquiterpenic alcohol
1-epi-Cubenol	0.03	Sesquiterpenic alcohol
Cubenol	0.03	Sesquiterpenic alcohol
(2 <i>Z</i> ,6 <i>Z</i>)-Farnesol	0.03	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	0.01	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.01	Sesquiterpenic aldehyde
Phytone	0.02	Terpenic ketone
Unknown	0.02	Unknown
Unknown	0.03	Unknown
Unknown	0.03	Unknown
Unknown	0.01	Unknown
Dicitral	0.04	Diterpenic aldehyde
Unknown	0.04	Unknown
Unknown	0.07	Unknown
Phytol isomer I	0.01	Diterpenic alcohol
Unknown	0.02	Unknown
Consolidated total	99.54	

tr: The compound has been detected below 0.005% of the total signal

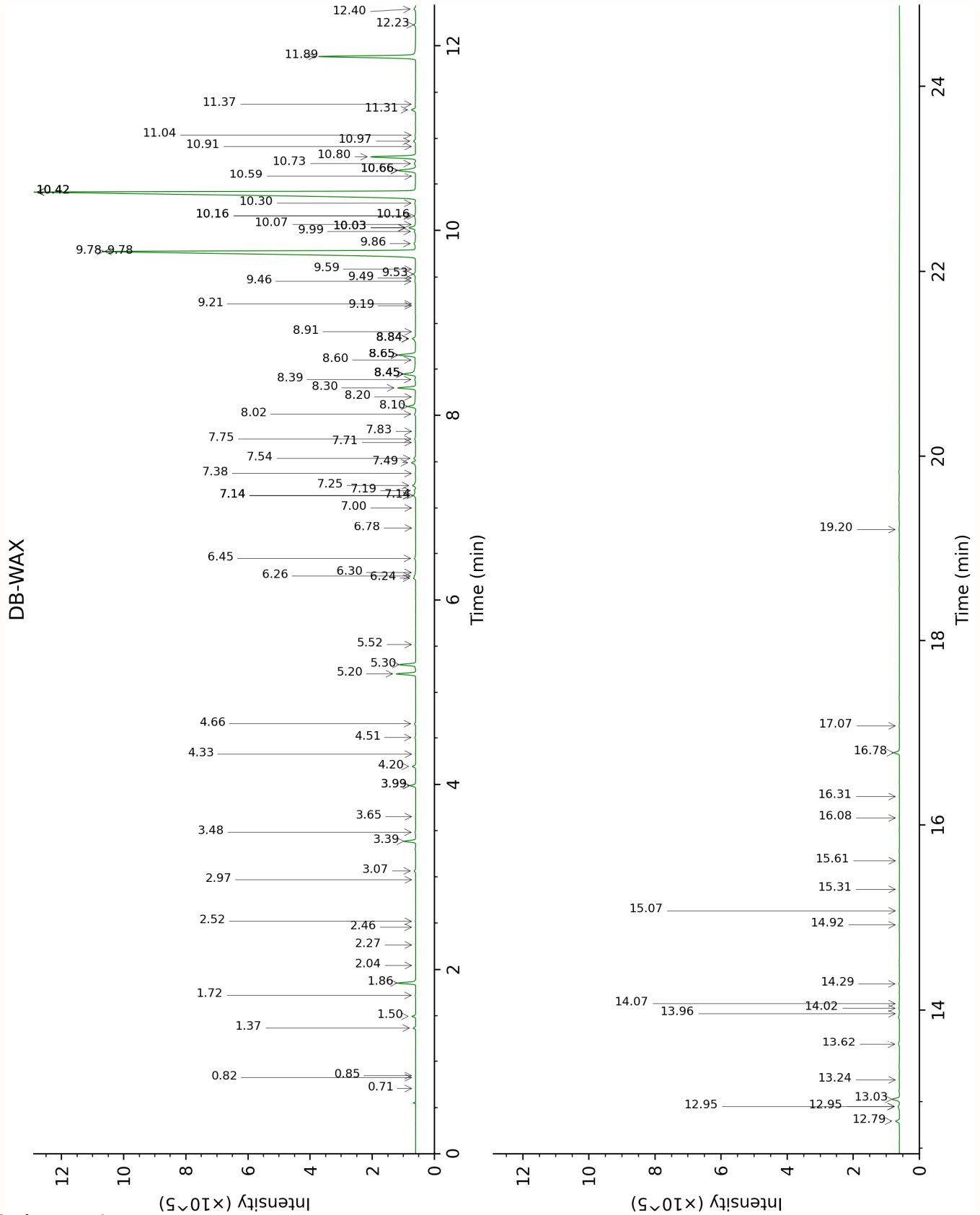
Note: no correction factor was applied

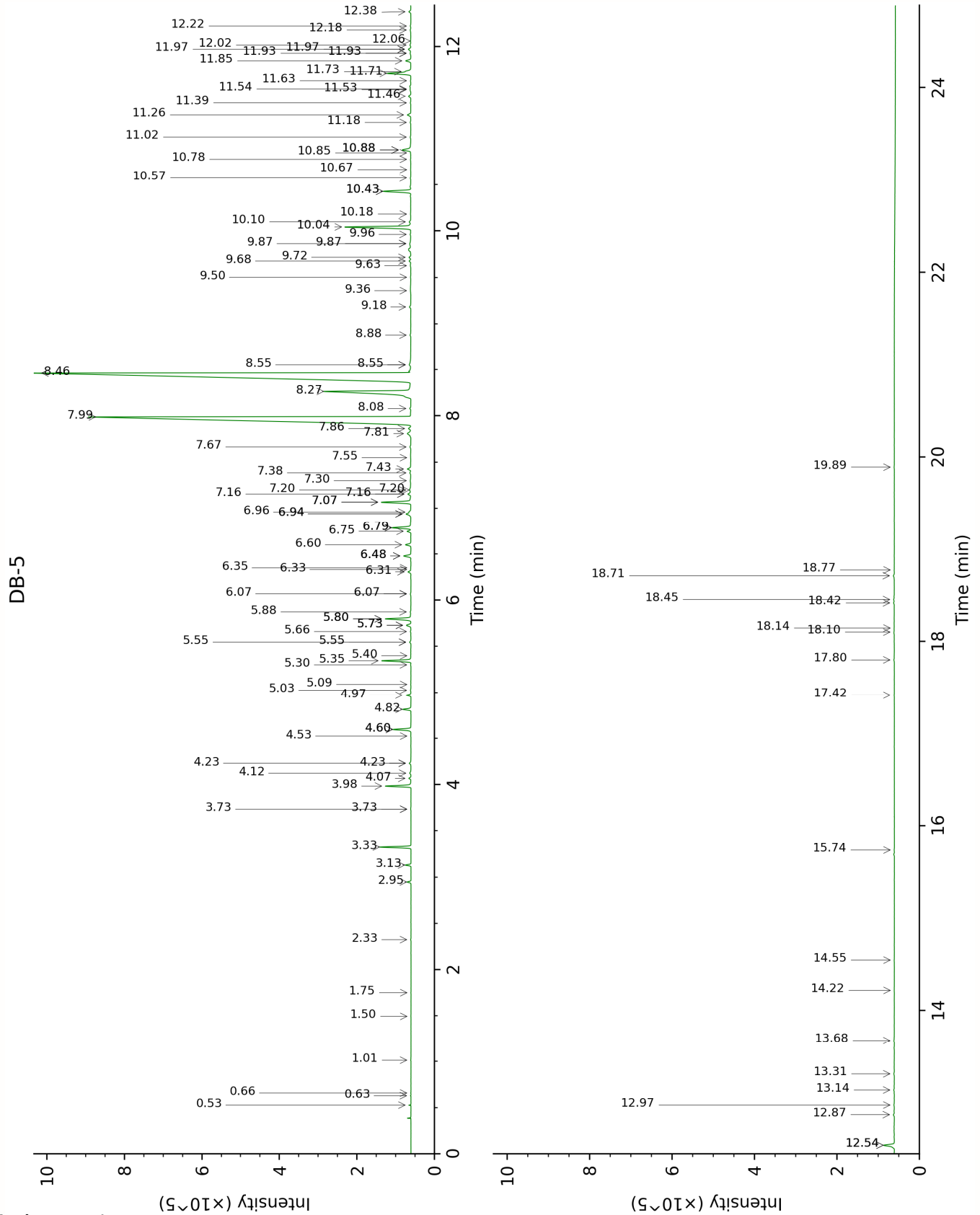
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm is set to prioritize data from the most standard DB-5 column, and smallest values so as to avoid overestimating individual content. This process is semi-automatic. Advanced users are invited to consult the "Full analysis data" table after the chromatograms in this report to access the full untreated data and perform their own calculations if needed.

Unknowns: Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

Bracketed value ([xx]): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

2-Methyl-3-buten-2-ol	Column DB-WAX			Column DB-5		
	1.72	1014.4	0.03	0.53	606.1	0.03
Isovaleral	0.85	886.6	0.01	0.63	641.4	0.01
2-Methylbutyral	0.82	879.1	tr	0.66	651.5	tr
Isoamyl alcohol	3.65	1177.4	0.02	1.02	733.1	0.01
Hexanal	2.04	1045.3	tr	1.50	800.6	0.01
Unknown PEGR III [m/z 81, 69 (80), 41 (65), 83 (52), 109 (48), 55 (47)...]	0.71	838.7	tr	1.75	823.5	tr
4-Heptanone	2.52	1090.7	0.02	2.32	871.1	0.02
Tricyclene	1.37	971.7	0.12	2.95	919.1	0.13
α -Pinene	1.50	991.3	0.18	3.13	931.2	0.18
Camphene	1.86	1027.2	1.02	3.33	944.2	1.03
Sabinene	2.46	1084.7	0.02	3.74*	971.2	[0.02]
β -Pinene	2.27	1066.5	0.01	3.74*	971.2	[0.02]
6-Methyl-5-hepten-2-one	5.30	1300.1	0.95	3.98	987.7	0.94
Myrcene	3.07	1133.1	0.08	4.07	993.2	0.09
6-Methyl-5-hepten-2-ol	7.14*	1430.4	[0.21]	4.12	996.9	0.08
Octanal	4.66	1249.1	0.07	4.23*	1004.1	[0.09]
α -Phellandrene	2.97	1125.8	0.01	4.23*	1004.1	[0.09]
<i>para</i> -Cymene	4.33	1226.0	0.02	4.52	1022.5	0.01
1,8-Cineole	3.48	1164.7	0.05	4.60*	1027.0	[0.69]
Limonene	3.39	1157.4	0.68	4.60*	1027.0	[0.69]
(Z)- β -Ocimene	3.99*	1202.1	[0.34]	4.82	1040.7	0.32
(E)- β -Ocimene	4.20	1216.7	0.20	4.97	1050.4	0.19
2,6-Dimethyl-5-heptenal (melonal)	5.52	1315.3	0.03	5.03	1054.0	0.04
γ -Terpinene	3.99*	1202.1	[0.34]	5.09	1057.9	0.01
<i>cis</i> -Linalool oxide (fur.)	6.78	1404.3	0.02	5.30	1071.3	0.02
4-Nonanone	5.20	1287.3	1.14	5.35	1074.1	1.10
Octanol	8.45*	1527.7	[1.10]	5.40	1077.4	0.02
Terpinolene	4.51	1238.6	0.05	5.55*	1086.6	[0.06]
<i>trans</i> -Linalool oxide (fur.)	7.14*	1430.4	[0.21]	5.55*	1086.6	[0.06]
4-Nonanol				5.66	1093.8	0.03
Rosefuran	6.24	1365.8	0.13	5.73*	1098.1	[0.23]
Perillene	6.30	1370.1	0.03	5.73*	1098.1	[0.23]
<i>cis</i> -	6.26	1367.5	0.10	5.80*	1102.5	[1.08]

Chrysanthemal?						
Linalool	8.30	1516.3	1.05	5.80*	1102.5	[1.08]
(Z)-6-Methyl-3,5-heptadien-2-one	8.45*	1527.7	[1.10]	5.88	1107.2	0.04
<i>trans-para</i> -Mentha-2,8-dien-1-ol	9.21	1585.9	0.02	6.07*	1119.7	[0.03]
Unknown CYFL II [m/z 81, 79 (19), 41 (12), 92 (8), 77 (8)...]	6.45	1380.9	0.09	6.07*	1119.7	[0.03]
Unknown CYFL III [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	7.14*	1430.4	[0.21]	6.31	1134.9	0.13
Unknown CYFL IV [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	7.83	1481.0	0.01	6.33	1136.5	0.01
<i>trans-para</i> -Menth-2-en-1-ol	9.19	1584.4	0.01	6.35	1137.7	0.01
<i>trans</i> -Chrysanthemal	7.49	1456.3	0.29	6.48*	1145.9	[0.34]
exo-Isocitral	7.75	1475.0	0.07	6.48*	1145.9	[0.34]
Citronellal	7.24	1438.3	0.24	6.60	1153.6	0.24
Borneol	10.03*	1651.1	[0.46]	6.75	1163.0	0.15
Isoneral	8.10	1500.9	0.63	6.79*	1165.5	[0.79]
α -Phellandren-8-ol	10.42*	1681.8	[41.80]	6.79*	1165.5	[0.79]
Terpinen-4-ol	8.84*	1557.3	[0.26]	6.94*	1175.4	[0.26]
Rosefuran oxide	8.84*	1557.3	[0.26]	6.94*	1175.4	[0.26]
Unknown CYFL V [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	9.86	1637.5	0.13	6.96	1176.6	0.10
Unknown CYFL XIV [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9)...]				7.07*	1183.5	[1.24]
Isogeranial	8.45*	1527.7	[1.10]	7.07*	1183.5	[1.24]
α -Terpineol	10.03*	1651.1	[0.46]	7.16*	1189.1	[0.16]
Myrtenal	8.91	1563.1	0.02	7.16*	1189.1	[0.16]

(4Z)-Decenal	8.02	1494.6	0.08	7.20*	1191.9	[0.13]
Unknown DRMO III [m/z 43, 81 (47), 67 (45), 69 944), 41 (42), 59 (40), 55 (39)...]	9.46	1605.0	0.06	7.20*	1191.9	[0.13]
<i>trans</i> - Isopiperitenol	10.66*	1701.5	[1.31]	7.30	1198.4	0.07
Unknown CYFL VI [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	10.42*	1681.8	[41.80]	7.38	1203.8	0.07
Decanal	7.54	1459.7	0.13	7.43	1206.5	0.18
<i>cis</i> - Isopiperitenol	10.59	1695.7	0.01	7.55	1214.7	0.01
2,3-Epoxyneral?				7.66	1222.5	0.05
Nerol	11.31	1756.3	0.28	7.81	1232.1	0.27
Citronellol	10.97	1728.0	0.12	7.86	1235.8	0.12
Neral	9.78*	1630.7	[31.81]	7.99	1244.3	31.73
Piperitone	10.16*	1661.2	[0.12]	8.08	1250.3	0.05
Geraniol	11.89	1805.3	6.27	8.27	1262.7	5.98
Geranial	10.42*	1681.8	[41.80]	8.46*†	1276.0	[41.67]
Bornyl acetate	8.45*	1527.7	[1.10]	8.55*†	1282.0	[0.15]
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	13.24	1925.5	0.02	8.55*†	1282.0	[0.15]
Geranyl formate	10.16*	1661.2	[0.12]	8.88	1303.9	0.04
Methyl geranate	9.99	1647.9	0.09	9.18	1325.3	0.07
Unknown CYFL VIII [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	12.95*	1899.1	[0.11]	9.36	1337.7	0.05
α -Cubebene	7.00	1420.6	0.01	9.50	1347.8	0.02
Citronellyl acetate	9.78*	1630.7	[31.81]	9.63	1356.7	0.03
Cyclosativene I	7.14*	1430.4	[0.21]	9.68	1360.2	0.07
Cyclosativene II	7.19	1434.3	0.10	9.72	1363.0	0.08
α -Copaene	7.38	1447.8	0.04	9.87*†	1373.4	[0.12]
Geranic acid				9.87*†	1373.4	[0.12]
β -Bourbonene	7.71	1472.2	0.03	9.96	1380.4	0.04

Geranyl acetate	10.80	1713.9	2.87	10.04	1386.1	2.83
β-Elemene	8.65*	1543.3	[1.28]	10.10	1390.0	0.08
Longifolene	8.20	1508.8	0.06	10.18	1395.8	0.03
β-Ylangene	8.39	1523.1	0.08	10.43*	1413.7	[1.19]
β-Caryophyllene	8.65*	1543.3	[1.28]	10.43*	1413.7	[1.19]
β-Copaene	8.60	1539.2	0.07	10.58	1424.6	0.03
<i>trans</i> -α-Bergamotene	8.65*	1543.3	[1.28]	10.67	1431.5	0.02
6,9-Guaiadiene	8.84*	1557.3	[0.26]	10.78	1439.9	0.03
<i>cis</i> -β-Bergamotene?				10.85	1445.1	0.02
α-Humulene	9.53	1611.2	0.14	10.88*	1447.5	[0.47]
(<i>E</i>)-Isoeugenol	16.78	2272.3	0.36	10.88*	1447.5	[0.47]
<i>cis</i> -Muurolo-4(15),5-diene	9.59	1615.5	0.03	11.02	1457.8	0.04
<i>trans</i> -Cadina-1(6),4-diene	9.49	1607.8	0.03	11.18	1469.6	0.03
Germacrene D	10.03*	1651.1	[0.46]	11.26	1475.7	0.17
γ-Amorphene	10.07	1653.9	0.02	11.39	1485.4	0.03
epi-Cubebol	12.23	1835.2	0.10	11.46	1490.7	0.11
α-Muurolene	10.30	1672.2	0.06	11.53	1496.0	0.04
Methyl (<i>E</i>)-isoeugenol	15.31	2121.9	0.02	11.54	1496.6	0.02
δ-Amorphene	10.16*	1661.2	[0.12]	11.63	1503.2	0.02
γ-Cadinene	10.66*	1701.5	[1.31]	11.71	1509.4	1.09
Cubebol	12.79	1884.8	0.24	11.73	1510.9	0.18
δ-Cadinene	10.66*	1701.5	[1.31]	11.85	1520.0	0.24
<i>trans</i> -Cadina-1,4-diene	10.92	1723.2	0.02	11.93*	1526.5	[0.05]
10-epi-Cubebol?	14.07	2002.3	0.03	11.93*	1526.5	[0.05]
(<i>E</i>)-γ-Bisabolene	10.73	1707.7	0.08	11.97*	1529.9	[0.12]
Unknown CYFL XV [m/z 85, 59 (82), 71 (58), 41 (36), 43 (34)...]				11.97*	1529.9	[0.12]
α-Cadinene	11.04	1733.4	0.04	12.02	1533.5	0.05
Neryl butyrate				12.06	1536.9	0.03
α-Elemol	14.28	2022.8	0.04	12.18	1546.2	0.04
Germacrene B	11.37	1761.4	0.04	12.22	1549.6	0.03
Geranyl butyrate	12.40	1850.4	0.13	12.38	1561.8	0.09
Caryophyllene oxide	13.03	1906.3	0.49	12.54*	1574.4	[0.52]
Caryophyllene oxide isomer	12.95*	1899.1	[0.11]	12.54*	1574.4	[0.52]
Humulene	13.62	1960.8	0.05	12.87	1600.4	0.05

epoxide II						
Selin-6-en-4 α -ol isomer	15.07	2098.8	0.02	12.97	1608.8	0.03
1-epi-Cubenol	14.02	1997.5	0.04	13.14	1622.3	0.03
Cubenol	13.96	1991.9	0.02	13.31	1636.8	0.03
(2Z,6Z)-Farnesol	16.31	2223.2	0.02	13.68	1666.9	0.03
(2E,6Z)-Farnesal	15.61	2152.6	0.01	14.22	1712.3	0.01
(2E,6E)-Farnesal	16.08	2199.2	0.02	14.55	1740.8	0.01
Phytone	14.92	2083.8	0.03	15.74	1846.0	0.02
Unknown LICU V [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]				17.42	2002.8	0.02
Unknown LICU VII [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]				17.80	2040.9	0.03
Unknown CYFL IX [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]				18.10	2070.8	0.03
Unknown LIMU XXI [m/z 57, 85 (55), 163 (47), 41 (44), 120 (35), 202 (30), 145 (25)... 219 (17), 304 (t)]				18.14	2075.2	0.01
Dicital	17.07	2303.2	0.02	18.42	2102.3	0.04
Unknown DRMO VI [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	19.20	2540.4	0.04	18.45	2105.9	0.04
Unknown LICU II [m/z 69, 41 (38), 151 (36), 123 (34), 82 (24), 43 (23), 109 (21)...]				18.71	2132.6	0.07
Phytol isomer I				18.77	2139.1	0.01
Unknown CYFL XII [m/z 123, 94				19.89	2257.1	0.02

(100), 43 (86), 69						
(75), 95 (47), 41						
(47), 93 (45)...						
Total reported	98.83%			99.37%		

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is taken into account in the consolidated total

†: Peaks apexes were resolved, but peaks overlapped and were summed for analysis

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index